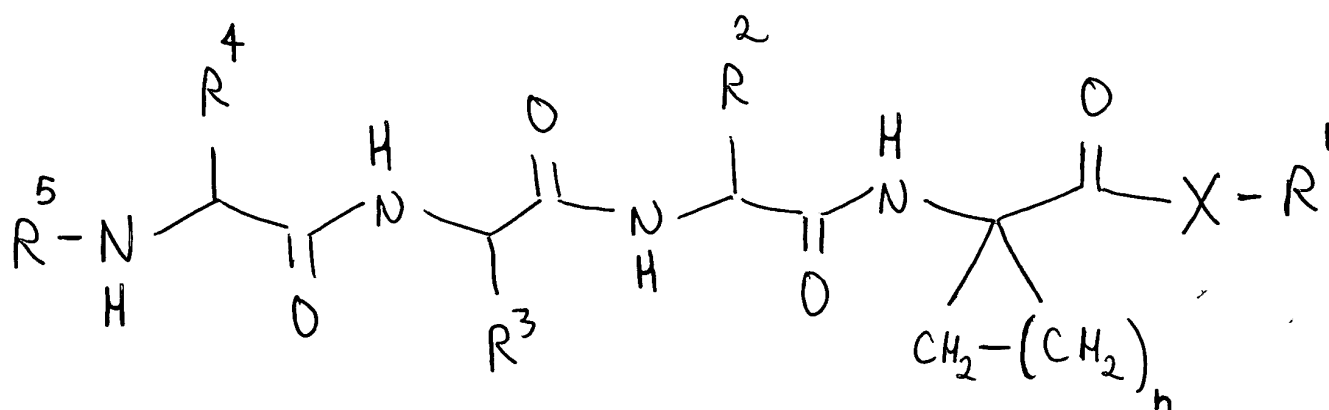


09/368 670





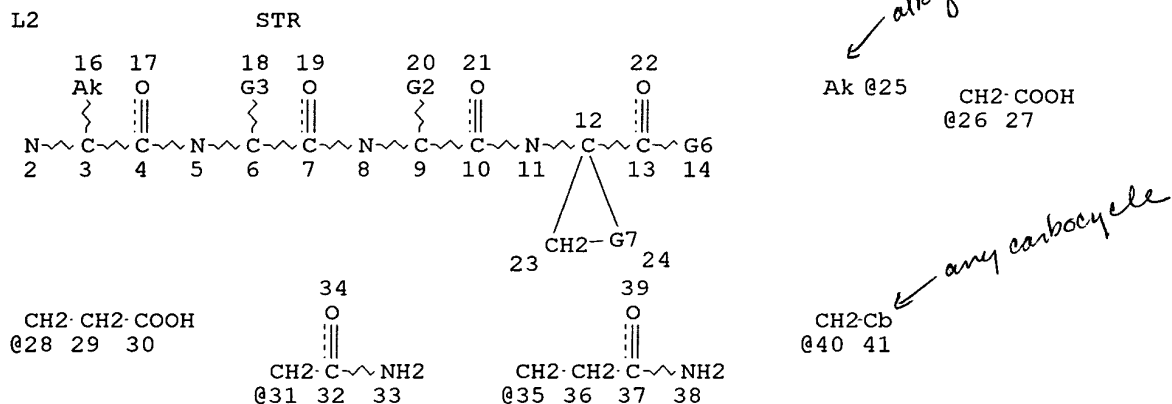
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 DICTIONARY FILE UPDATES: 16 FEB 2000 HIGHEST RN 256241-24-4

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 13, 1999

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VAR G2=25/40/26/28/31/35

VAR G3=25/26/28

VAR G6=NH/O

REP G7=(1-4) C

NODE ATTRIBUTES:

CONNECT IS E1 RC AT 16

CONNECT IS E1 RC AT 25

DEFAULT MLEVEL IS ATOM

GGCAT IS MCY UNS AT 41

DEFAULT ECLEVEL IS LIMITED

ECOUNT IS E6 C AT 41

*carbocycle at 41 is monocyclic, unsaturated  
 & has exactly 6 carbons*

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 39

STEREO ATTRIBUTES: NONE

L4 32 SEA FILE=REGISTRY SSS FUL L2

100.0% PROCESSED 1093 ITERATIONS

SEARCH TIME: 00.00.01

32 ANSWERS

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 PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

Searched by Barb O'Bryen, STIC 308-4291

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FILE COVERS 1967 - 17 Feb 2000 VOL 132 ISS 8  
FILE LAST UPDATED: 16 Feb 2000 (20000216/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

This file supports REGISTRY for direct browsing and searching of all substance data from the REGISTRY file. Enter HELP FIRST for more information.

L2 STR  
L4 32 SEA FILE=REGISTRY SSS FUL L2  
L5 8 SEA FILE=CAPLUS ABB=ON L4

=> d ibib abs hitstr l5 1-8

L5 ANSWER 1 OF 8 CAPLUS COPYRIGHT 2000 ACS  
ACCESSION NUMBER: 1999:682201 CAPLUS  
DOCUMENT NUMBER: 132:78839  
TITLE: Long-range electron transfer in rigid 310-helical  
oligopeptides containing redox cyclic .alpha.-amino  
acids  
AUTHOR(S): Lang, Kamil; Kuki, Atsuo  
CORPORATE SOURCE: Department of Chemistry, University of California,  
Santa Cruz, CA, USA  
SOURCE: Photochem. Photobiol. (1999), 70(4), 579-584  
CODEN: PHCBAP; ISSN: 0031-8655  
PUBLISHER: American Society for Photobiology  
DOCUMENT TYPE: Journal  
LANGUAGE: English

AB Intrahelical photoinduced electron transfer processes (ET) in conformationally restricted oligopeptides have been studied by nanosecond time-resolved transient spectroscopy. The helical peptides were constructed from sterically hindered .alpha.-aminoisobutyric acid (Aib) and two cyclic .alpha.-amino acids (Aib class) bearing electron acceptor and donor side chains (DkNap, ThQx). This helical backbone design provides high conformation stability, as previously demonstrated, and yields reliable 310-helical architectures in soln. The forward ET between ThQx and 3DkNap is followed by a slow back ET thus giving rise to an accumulation of the charge-sepd. ion pairs for hundreds of nanoseconds. We demonstrate the modulation of electronic interactions by the no. of intervening Aib residues sepg. acceptor-donor side chains and propose modifications of the peptide framework by inclusion of a non-Aib amino acid residue. These well-defined and sterically stable frameworks are suited for the precise evaluation of intrahelical electron transfer processes mediated by peptides.

IT 253670-46-1P 253670-47-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)  
(prepn. and reaction of in the synthesis of rigid 310-helical  
oligopeptides contg. redox cvcltic .alpha.-amino acids for study of  
Searched by Barb O'Bryen, STIC 308-4291

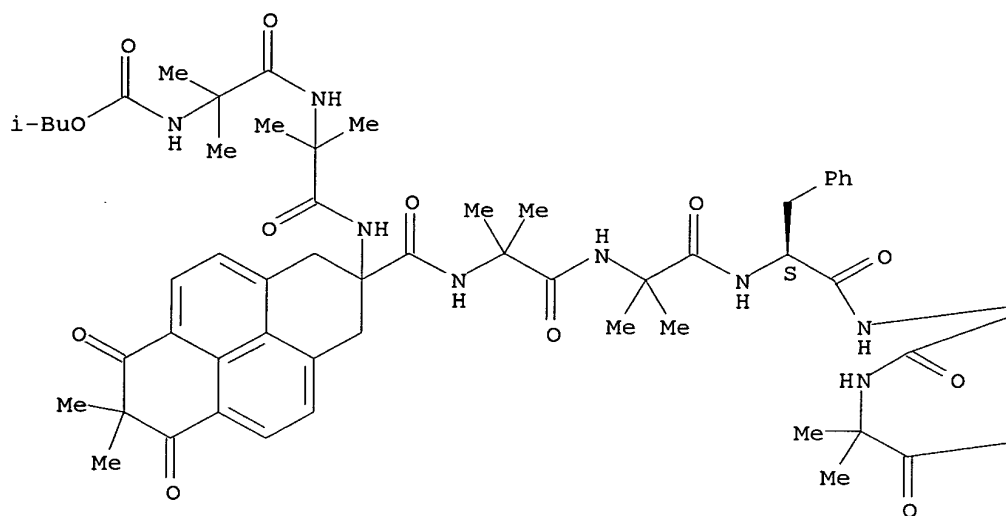
long-range electron transfer)

RN 253670-46-1 CAPLUS

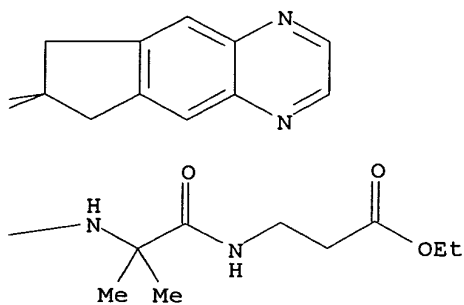
CN .beta.-Alanine, 2-methyl-N-[(2-methylpropoxy)carbonyl]alanyl-2-methylalanyl-2-amino-1,2,3,6,7,8-hexahydro-7,7-dimethyl-6,8-dioxo-2-pyrenecarbonyl-2-methylalanyl-2-methylalanyl-L-phenylalanyl-7-amino-7,8-dihydro-6H-cyclopenta[g]quinoxaline-7-carbonyl-2-methylalanyl-2-methylalanyl-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



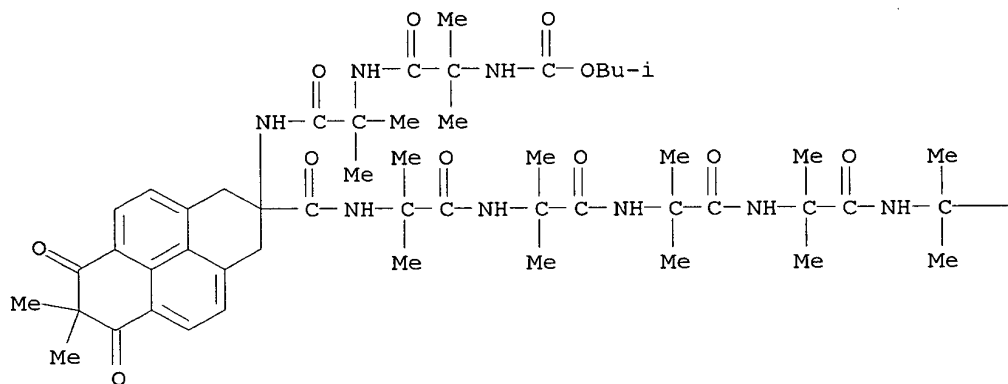
RN 253670-47-2 CAPLUS

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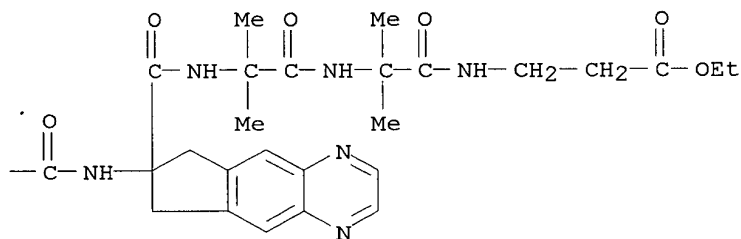
Searched by Barb O'Bryen, STIC 308-4291

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2-methylalanyl-7-amino-7,8-dihydro-6H-cyclopenta[g]quinoxaline-7-carbonyl-  
2-methylalanyl-2-methylalanyl-, ethyl ester (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 1-B



IT 253670-48-3P 253670-49-4P

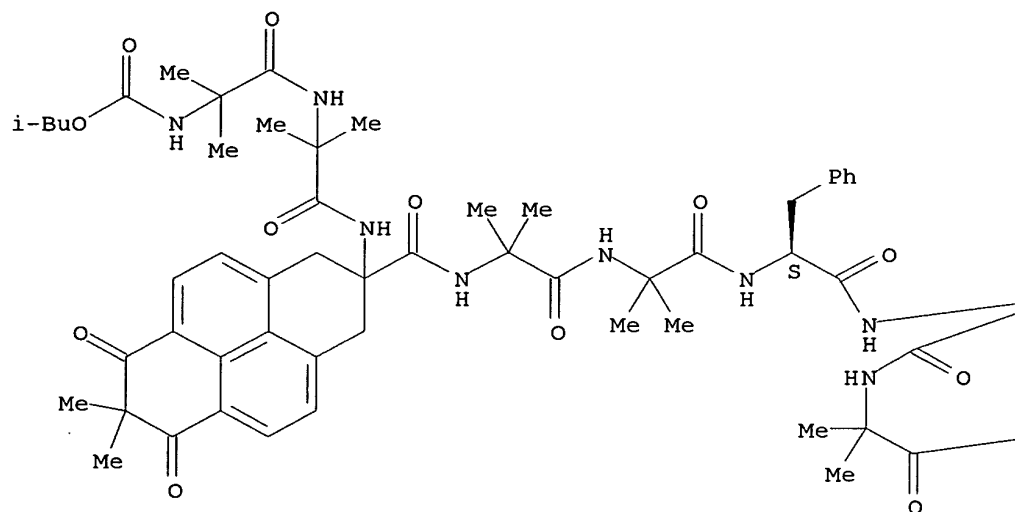
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.alpha.-amino acids for study of long-range electron transfer)

RN 253670-48-3 CAPLUS

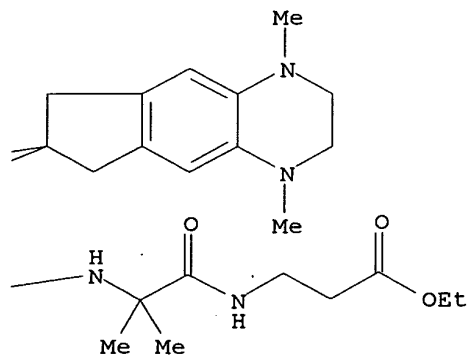
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pyrenecarbonyl-2-methylalanyl-2-methylalanyl-L-phenylalanyl-7-amino-  
2,3,4,6,7,8-hexahydro-1,4-dimethyl-1H-cyclopenta[g]quinoxaline-7-carbonyl-  
2-methylalanyl-2-methylalanyl-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

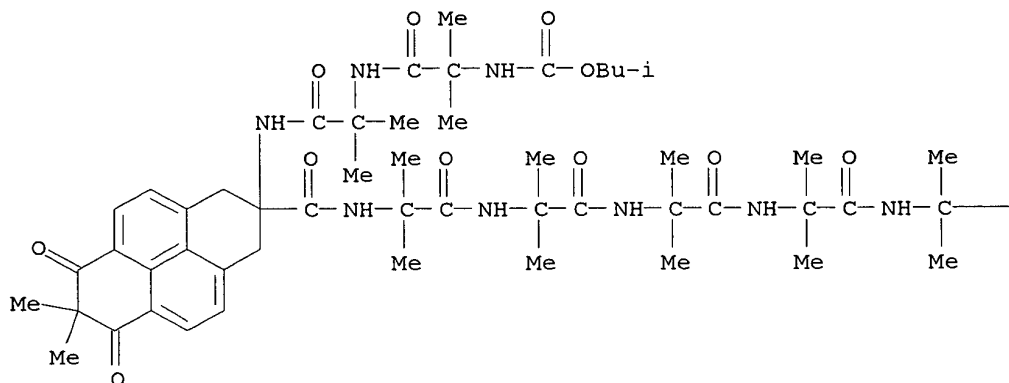


PAGE 1-B

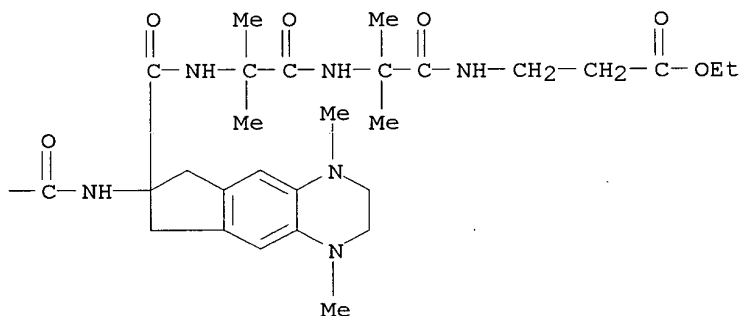


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PAGE 1-A



PAGE 1-B



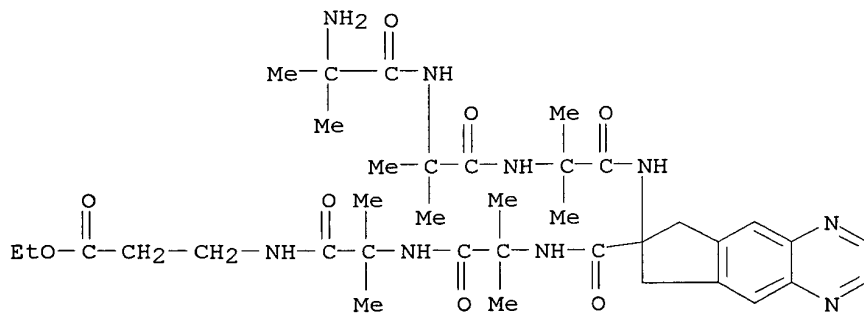
IT 253670-44-9

RL: RCT (Reactant)

(reaction of in the synthesis of rigid 310-helical oligopeptides contg.  
redox cyclic .alpha.-amino acids for study of long-range electron  
transfer)

RN 253670-44-9 CAPLUS

CN .beta.-Alanine, 2-methylalanyl-2-methylalanyl-2-methylalanyl-7-amino-7,8-  
dihydro-6H-cyclopenta[g]quinoxaline-7-carbonyl-2-methylalanyl-2-  
methylalanyl-, ethyl ester (9CI) (CA INDEX NAME)



Searched by Barb O'Bryen, STIC 308-4291



LS ANSWER 2 OF 8 CAPLUS COPYRIGHT 2000 ACS

ACCESSION NUMBER: 1997:707601 CAPLUS

DOCUMENT NUMBER: 128:18385

TITLE: Libraries of opiate and anti-opiate peptidomimetics containing 2,3-methanoleucine

AUTHOR(S): Burgess, Kevin; Li, Wen; Linthicum, D. Scott; Ni, Qing; Pledger, David; Rothman, Richard B.; Shitangkoon, Aroonsiri

CORPORATE SOURCE: Department of Chemistry, Texas AandM University, College Station, TX, 77843-3255, USA

SOURCE: Bioorg. Med. Chem. (1997), 5(9), 1867-1871  
CODEN: BMECEP; ISSN: 0968-0896

PUBLISHER: Elsevier

DOCUMENT TYPE: Journal

LANGUAGE: English

AB A library of 96 peptides/peptidomimetics was prepd., in which half was based on the YGGFL-NH2 sequence, while the remainder were derivs. of a presumed anti-opiate peptide, YGGFLRF-NH2. Of the 48 compds. in each half of the library, 32 contained a stereoisomer of 2,3-methanoleucine substituted for Leu5. Binding of the YGGFL-NH2 derivs. to the .mu.-and .delta.-opioid receptors, and to the anti-.beta.-endorphin monoclonal antibody (clone 3E7), indicated any change at the Leu5 had little effect on the binding when compared with modifications to the YGGF-sequence. Conversely, cyclo-Leu residues did alter the binding of YGGFLRF-NH2 derivs. when substituted for Leu5. Of these 32 peptidomimetics, three derivs. of 2S,3S-cyclo-Leu had relatively low Ki values for binding to an NPFF receptor. Differences between the outcome of the screens were interpreted in terms of the position of the cyclo-Leu residue in the two sequences.

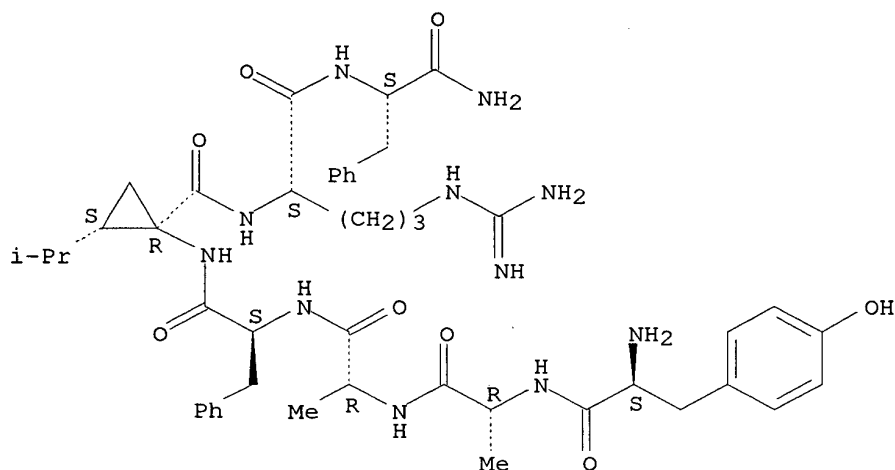
IT 185751-47-7 185751-51-3 185751-55-7  
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199445-05-1 199445-06-2 199445-07-3  
199445-29-9 199445-31-3 199445-32-4  
199445-33-5

RL: BAC (Biological activity or effector, except adverse); PRP (Properties); BIOL (Biological study)  
(libraries of opiate and anti-opiate peptidomimetics contg. 2,3-methanoleucine)

RN 185751-47-7 CAPLUS

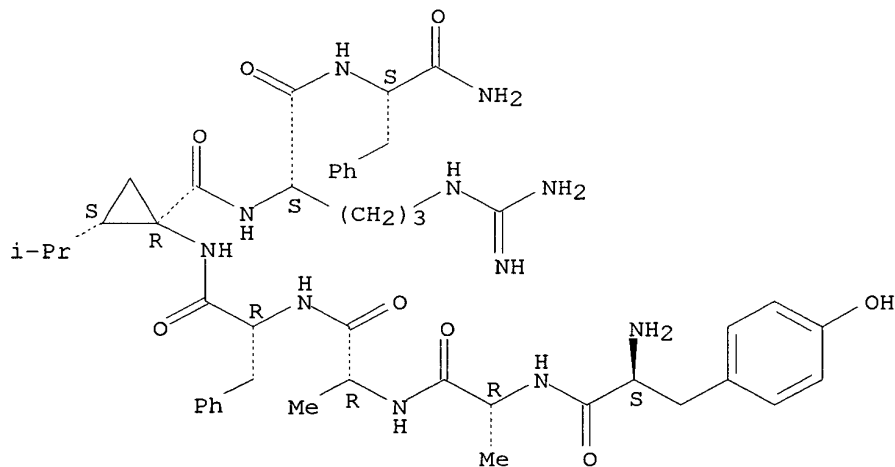
CN L-Phenylalaninamide, L-tyrosyl-D-alanyl-D-alanyl-L-phenylalanyl-(1R,2S)-1-amino-2-(1-methylethyl)cyclopropanecarbonyl-L-arginyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



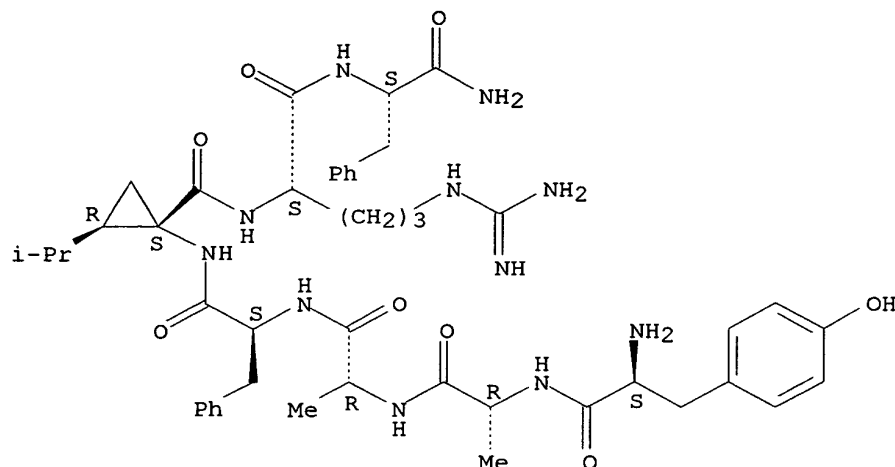
RN 185751-51-3 CAPLUS  
 CN L-Phenylalaninamide, L-tyrosyl-D-alanyl-D-alanyl-D-phenylalanyl-(1R,2S)-1-amino-2-(1-methylethyl)cyclopropanecarbonyl-L-arginyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 185751-55-7 CAPLUS  
 CN L-Phenylalaninamide, L-tyrosyl-D-alanyl-D-alanyl-L-phenylalanyl-(1S,2R)-1-amino-2-(1-methylethyl)cyclopropanecarbonyl-L-arginyl- (9CI) (CA INDEX NAME)

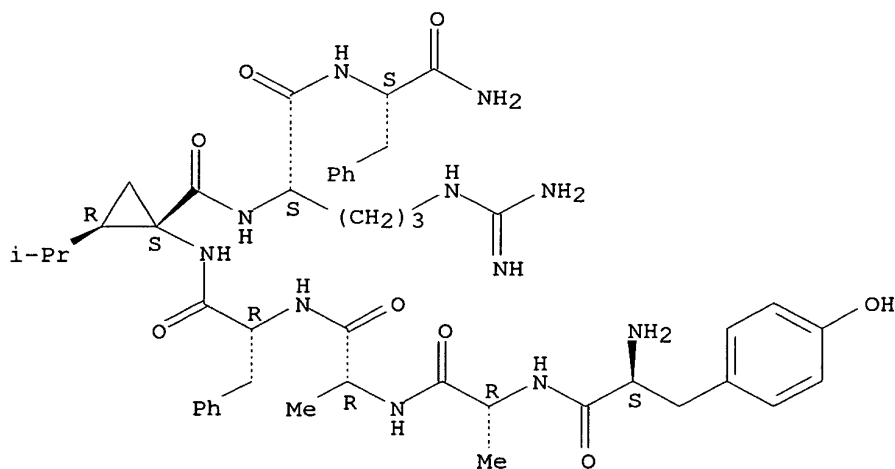
Absolute stereochemistry.



RN 185751-59-1 CAPLUS

CN L-Phenylalaninamide, L-tyrosyl-D-alanyl-D-alanyl-D-phenylalanyl-(1S,2R)-1-amino-2-(1-methylethyl)cyclopropanecarbonyl-L-arginyl- (9CI) (CA INDEX NAME)

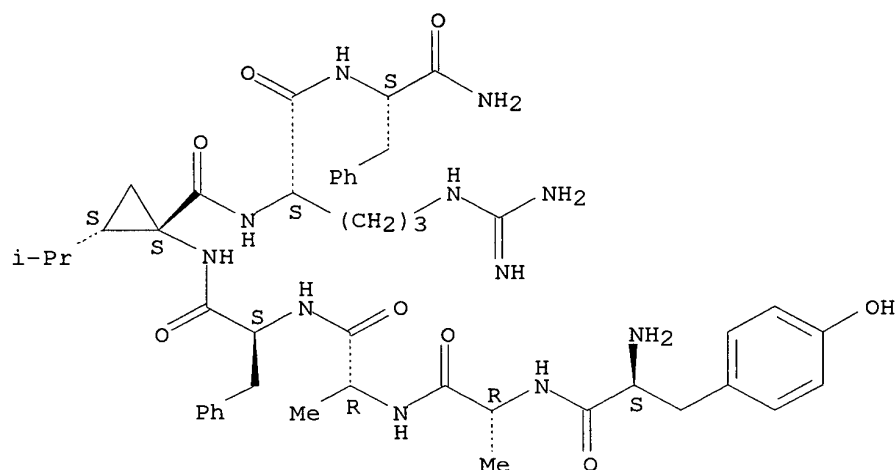
Absolute stereochemistry.



RN 185751-63-7 CAPLUS

CN L-Phenylalaninamide, L-tyrosyl-D-alanyl-D-alanyl-L-phenylalanyl-(1S,2S)-1-amino-2-(1-methylethyl)cyclopropanecarbonyl-L-arginyl- (9CI) (CA INDEX NAME)

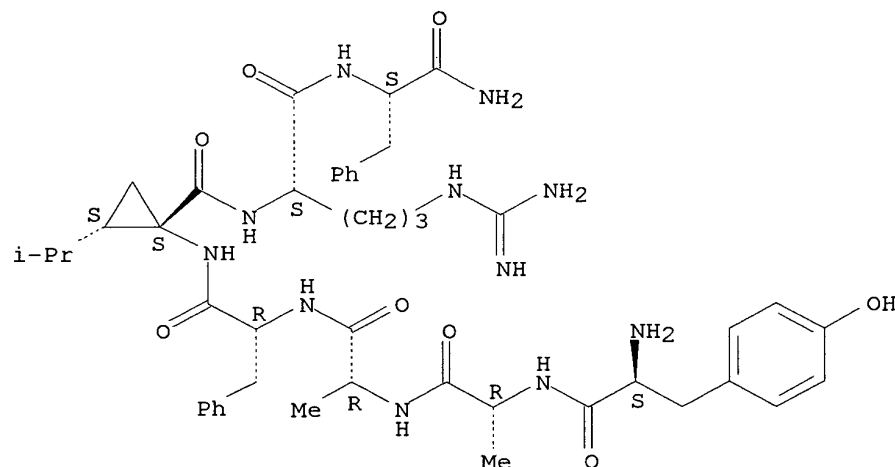
Absolute stereochemistry.



RN 185751-67-1 CAPLUS

CN L-Phenylalaninamide, L-tyrosyl-D-alanyl-D-alanyl-D-phenylalanyl-(1S,2S)-1-amino-2-(1-methylethyl)cyclopropanecarbonyl-L-arginyl- (9CI) (CA INDEX NAME)

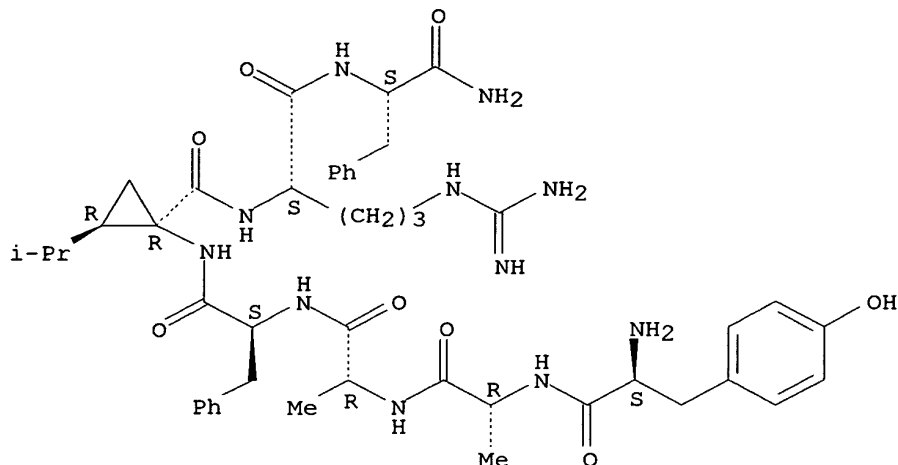
Absolute stereochemistry.



RN 185751-71-7 CAPLUS

CN L-Phenylalaninamide, L-tyrosyl-D-alanyl-D-alanyl-L-phenylalanyl-(1R,2R)-1-amino-2-(1-methylethyl)cyclopropanecarbonyl-L-arginyl- (9CI) (CA INDEX NAME)

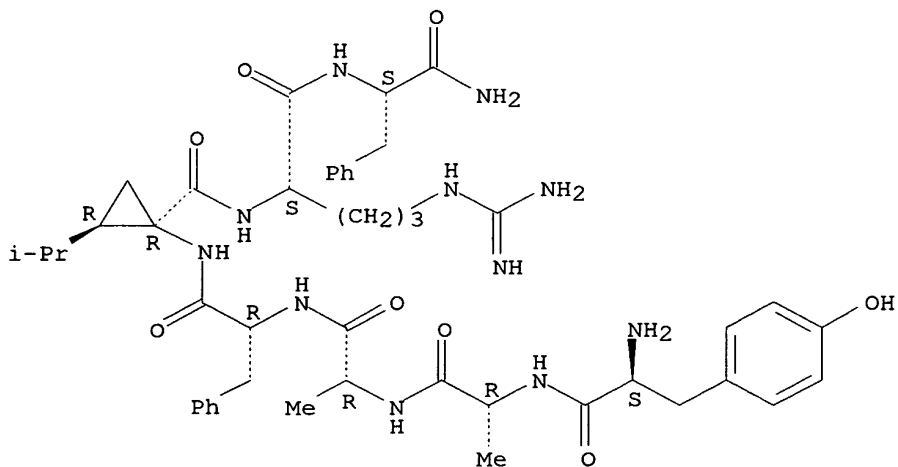
Absolute stereochemistry.



RN 185751-75-1 CAPLUS

CN L-Phenylalaninamide, L-tyrosyl-D-alanyl-D-alanyl-D-phenylalanyl-(1R,2R)-1-amino-2-(1-methylethyl)cyclopropanecarbonyl-L-arginyl- (9CI) (CA INDEX NAME)

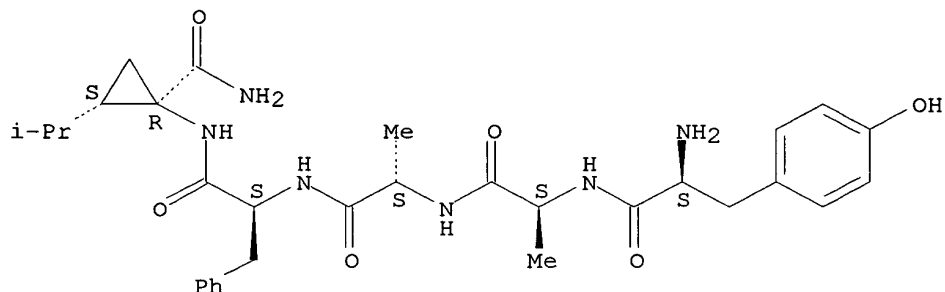
Absolute stereochemistry.



RN 199445-04-0 CAPLUS

CN Cyclopropanecarboxamide, L-tyrosyl-L-alanyl-L-alanyl-L-phenylalanyl-1-amino-2-(1-methylethyl)-, (1R,2S)- (9CI) (CA INDEX NAME)

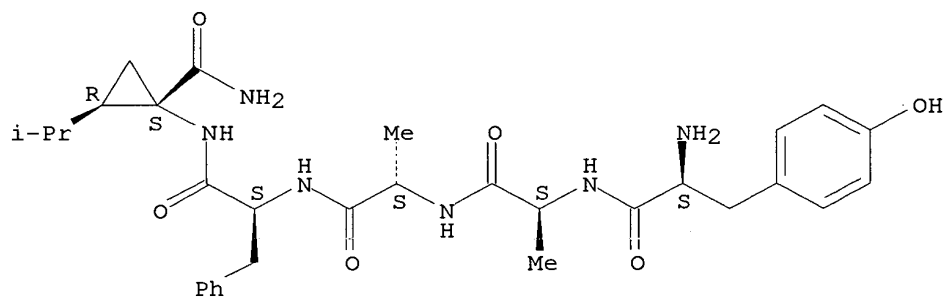
Absolute stereochemistry.



RN 199445-05-1 CAPLUS

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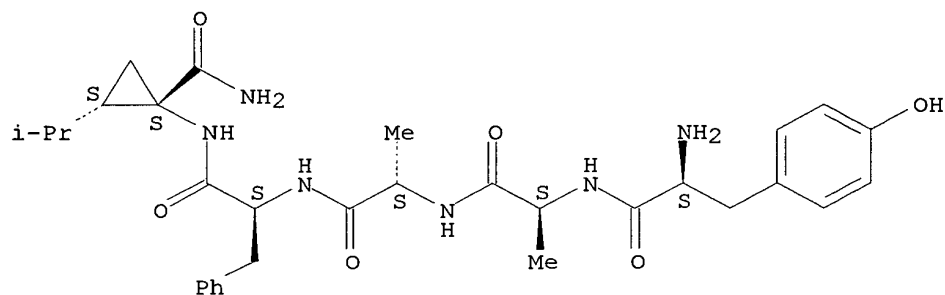
Absolute stereochemistry.



RN 199445-06-2 CAPLUS

CN Cyclopropanecarboxamide, L-tyrosyl-L-alanyl-L-alanyl-L-phenylalanyl-1-amino-2-(1-methylethyl)-, (1S,2S)- (9CI) (CA INDEX NAME)

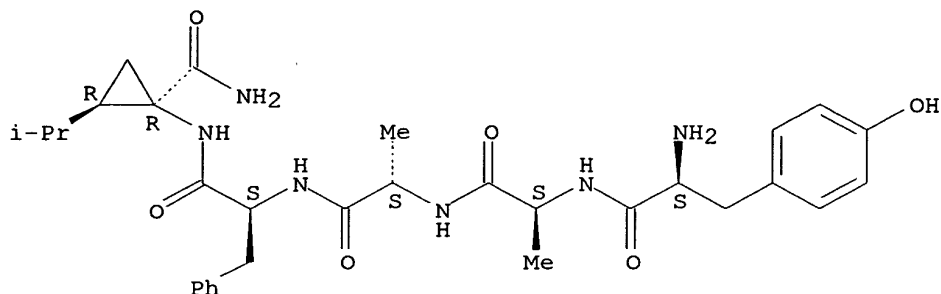
Absolute stereochemistry.



RN 199445-07-3 CAPLUS

CN Cyclopropanecarboxamide, L-tyrosyl-L-alanyl-L-alanyl-L-phenylalanyl-1-amino-2-(1-methylethyl)-, (1R,2R)- (9CI) (CA INDEX NAME)

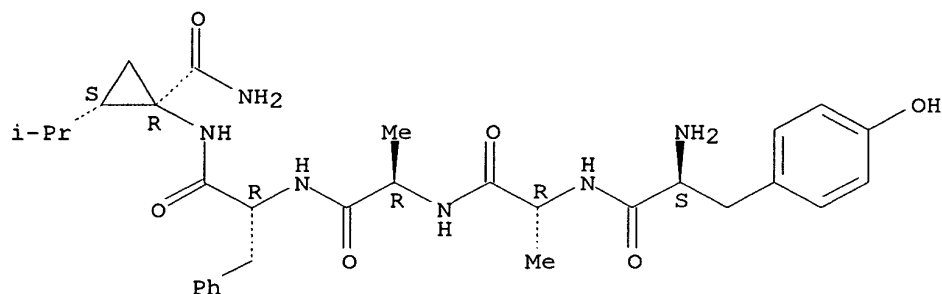
Absolute stereochemistry.



RN 199445-29-9 CAPLUS

CN Cyclopropanecarboxamide, L-tyrosyl-D-alanyl-D-alanyl-D-phenylalanyl-1-amino-2-(1-methylethyl)-, (1R,2S)- (9CI) (CA INDEX NAME)

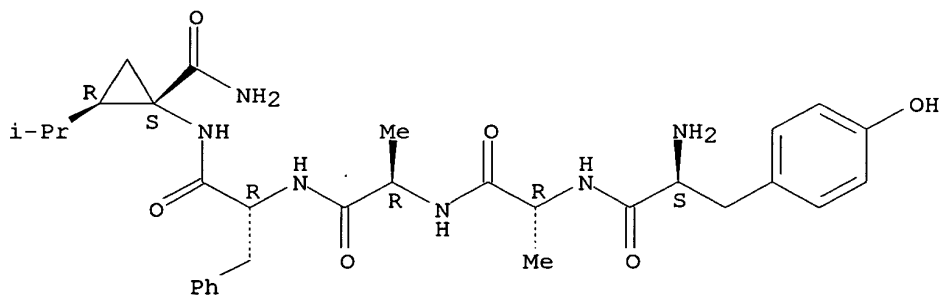
Absolute stereochemistry.



RN 199445-31-3 CAPLUS

CN Cyclopropanecarboxamide, L-tyrosyl-D-alanyl-D-alanyl-D-phenylalanyl-1-amino-2-(1-methylethyl)-, (1S,2R)- (9CI) (CA INDEX NAME)

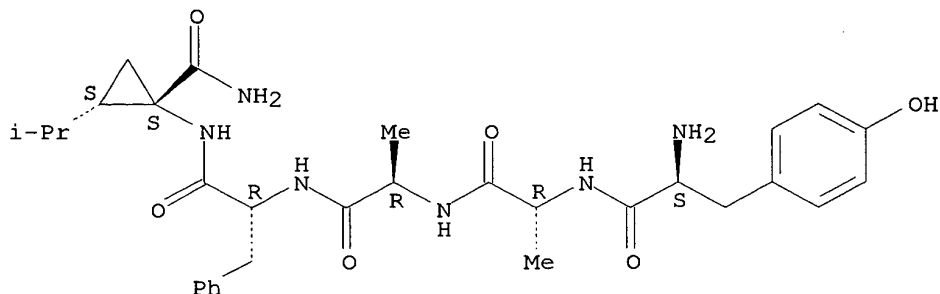
Absolute stereochemistry.



RN 199445-32-4 CAPLUS

CN Cyclopropanecarboxamide, L-tyrosyl-D-alanyl-D-alanyl-D-phenylalanyl-1-amino-2-(1-methylethyl)-, (1S,2S)- (9CI) (CA INDEX NAME)

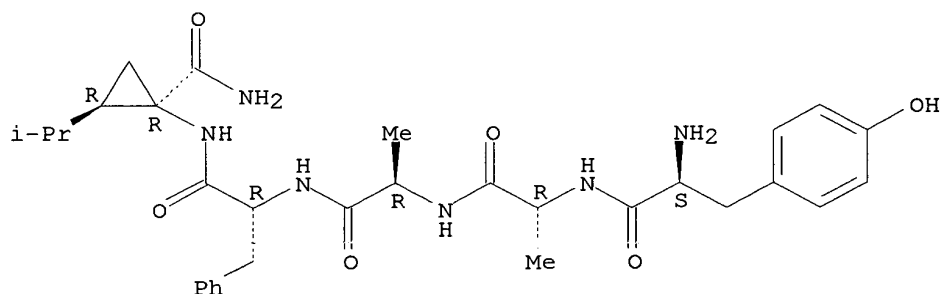
Absolute stereochemistry.



RN 199445-33-5 CAPLUS

CN Cyclopropanecarboxamide, L-tyrosyl-D-alanyl-D-alanyl-D-phenylalanyl-1-amino-2-(1-methylethyl)-, (1R,2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 3 OF 8 CAPLUS COPYRIGHT 2000 ACS

ACCESSION NUMBER: 1997:646051 CAPLUS

DOCUMENT NUMBER: 127:307651

TITLE: Design and synthesis of novel nonpolar host peptides for the determination of the 310- and .alpha.-helix compatibilities of .alpha.-amino acid building blocks: an assessment of .alpha.,.alpha.-disubstituted glycines

AUTHOR(S): Obrecht, Daniel; Altorfer, Michael; Bohdal, Udo; Daly, John; Huber, Walter; Labhardt, Alexander; Lehmann, Christian; Muller, Klaus; Ruffieux, Ruth; Schonholzer, Peter; Spiegler, Clive; Zumbrunn, Cornelia

CORPORATE SOURCE: F. Hoffmann-La Roche AG, Pharma Research, Basel, CH-4070, Switz.

SOURCE: Biopolymers (1997), 42(5), 575-626

CODEN: BIPMAA; ISSN: 0006-3525

PUBLISHER: Wiley

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The present work describes three novel nonpolar host peptide sequences that provide a ready assessment of the 310- and .alpha.-helix compatibilities of natural and unnatural amino acids at different positions of small- to medium-size peptides. The unpolar peptides contg. Ala, .alpha.-aminoisobutyric acid (Aib), and a C-terminal p-iodoanilide group were designed in such a way that the peptides could be rapidly assembled in a modular fashion, were highly sol. in solvent mixts. of trifluoroethanol and H<sub>2</sub>O for CD and two-dimensional NMR analyses, and showed excellent crystallinity suited for x-ray structure anal. To

Searched by Barb O'Bryen, STIC 308-4291



validate this approach, 9-mer peptides, 12-mer peptides, and 10-mer peptides incorporating a series of optically pure cyclic and open-chain (R)- and (S)-.alpha.,.alpha.-disubstituted glycines were prep'd. These amino acids are known to significantly modulate the conformations of small peptides. Based on x-ray structures, CD spectra recorded in acidic, neutral, and basic media and detailed 2D-NMR analyses, several interesting conformational observations were made. Esp. interesting results were obtained using the convex constraint CD anal. proposed by Fasman, which allowed the detn. of the relative content of 310- and .alpha.-helical conformations. These results were fully supported by the corresponding x-ray and 2D-NMR analyses. As a striking example, it was found that the (S)- and (R)-.beta.-tetralin derived amino acids show excellent .alpha.-helix stabilization, more pronounced than Aib and Ala. These novel ref. peptide sequences should help establish a scale for natural and unnatural amino acids concerning their intrinsic 310- and .alpha.-helix compatibilities at different positions of medium-sized peptides and thus improve the understanding of folding processes in peptides.

IT 197380-57-7P 197380-58-8P 197380-59-9P  
197380-60-2P 197381-27-4P 197381-29-6P  
197431-13-3P

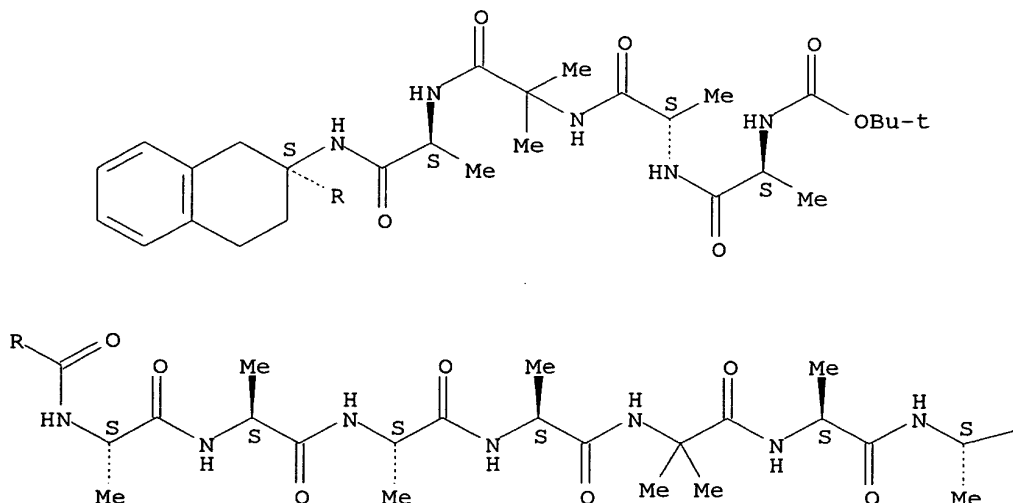
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
(design and synthesis of novel nonpolar host peptides for the detn. of  
the 310- and .alpha.-helix compatibilities of disubstituted glycine  
building blocks)

RN 197380-57-7 CAPLUS

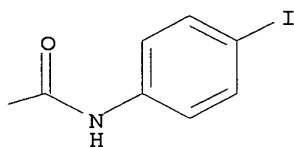
CN L-Alaninamide, N-[(1,1-dimethylethoxy)carbonyl]-L-alanyl-L-alanyl-2-methylalanyl-L-alanyl-(2S)-2-amino-1,2,3,4-tetrahydro-2-naphthalenecarbonyl-L-alanyl-L-alanyl-L-alanyl-L-alanyl-2-methylalanyl-L-alanyl-N-(4-iodophenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

PAGE 1-A



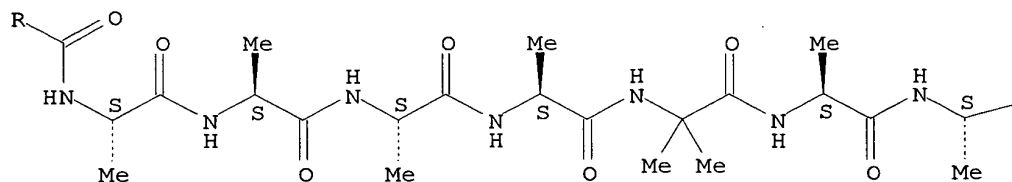
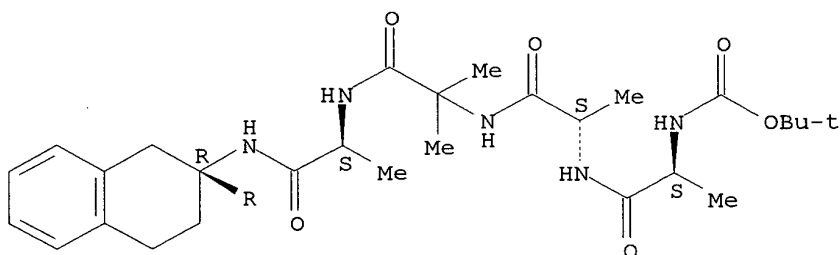
PAGE 1-B



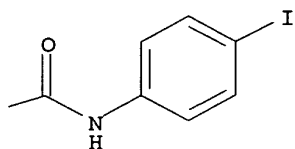
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 CN L-Alaninamide, N-[(1,1-dimethylethoxy)carbonyl]-L-alanyl-L-alanyl-2-methylalanyl-L-alanyl-(2R)-2-amino-1,2,3,4-tetrahydro-2-naphthalenecarbonyl-L-alanyl-L-alanyl-L-alanyl-L-alanyl-2-methylalanyl-L-alanyl-N-(4-iodophenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B

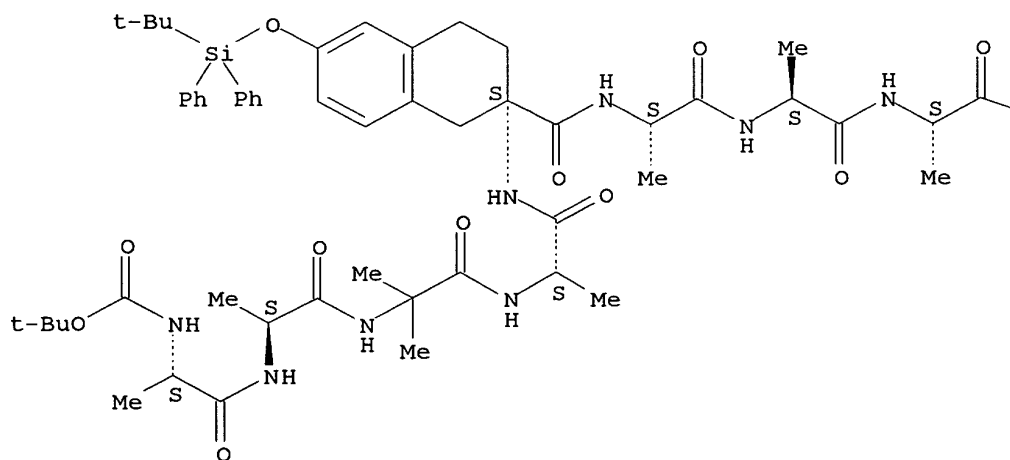


RN 197380-59-9 CAPLUS

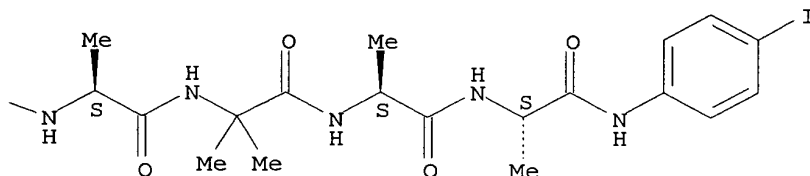
CN L-Alaninamide, N-[(1,1-dimethylethoxy)carbonyl]-L-alanyl-L-alanyl-2-methylalanyl-L-alanyl-(2S)-2-amino-6-[[[(1,1-dimethylethyl)diphenylsilyl]oxy]-1,2,3,4-tetrahydro-2-naphthalenecarbonyl]-L-alanyl-L-alanyl-L-alanyl-L-alanyl-2-methylalanyl-L-alanyl-N-(4-iodophenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

PAGE 1-A



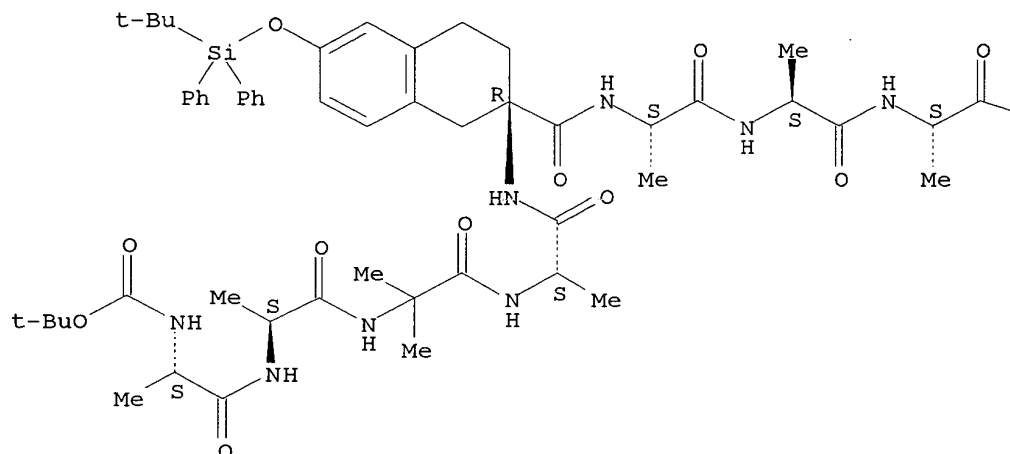
PAGE 1-B



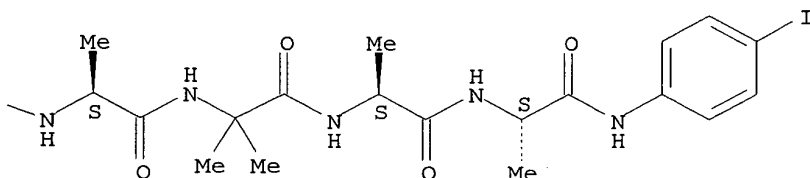
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 CN L-Alaninamide, N-[(1,1-dimethylethoxy)carbonyl]-L-alanyl-L-alanyl-2-methylalanyl-L-alanyl-(2R)-2-amino-6-[[ (1,1-dimethylethyl)diphenylsilyl]oxy]-1,2,3,4-tetrahydro-2-naphthalenecarbonyl-L-alanyl-L-alanyl-L-alanyl-L-alanyl-2-methylalanyl-L-alanyl-N-(4-iodophenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

PAGE 1-A



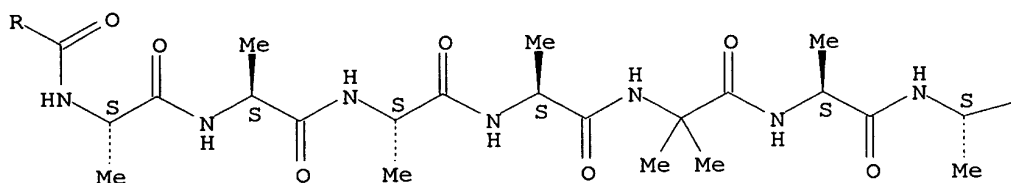
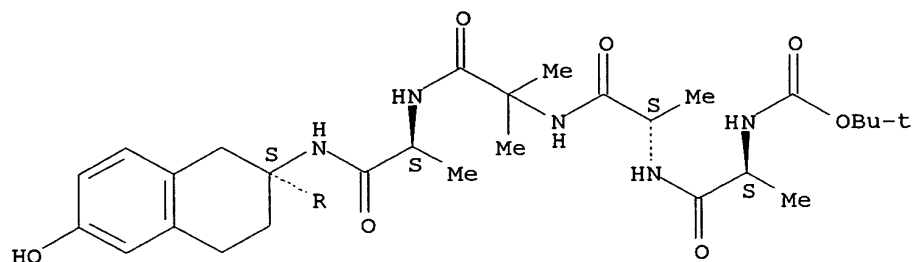
PAGE 1-B



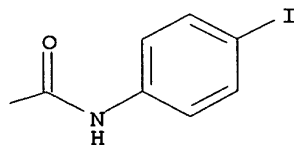
RN 197381-27-4 CAPLUS  
 CN L-Alaninamide, N-[(1,1-dimethylethoxy)carbonyl]-L-alanyl-L-alanyl-2-methylalanyl-L-alanyl-(2S)-2-amino-1,2,3,4-tetrahydro-6-hydroxy-2-naphthalenecarbonyl-L-alanyl-L-alanyl-L-alanyl-L-alanyl-2-methylalanyl-L-alanyl-N-(4-iodophenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).  
 Searched by Barb O'Bryen, STIC 308-4291

PAGE 1-A



PAGE 1-B

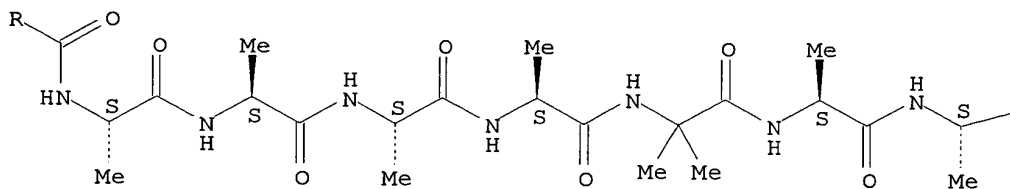
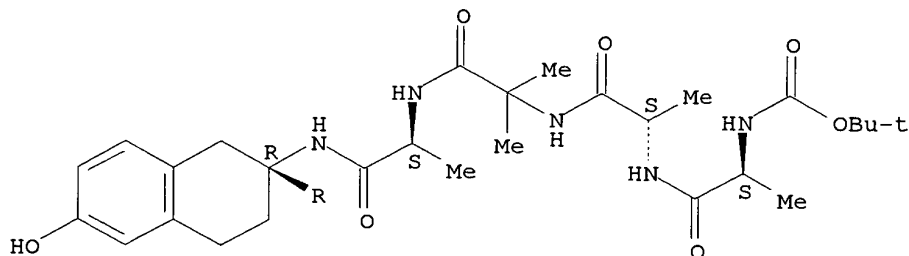


RN 197381-29-6 CAPLUS

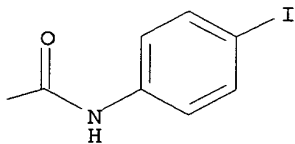
CN L-Alaninamide, N-[(1,1-dimethylethoxy)carbonyl]-L-alanyl-L-alanyl-2-methylalanyl-L-alanyl-(2R)-2-amino-1,2,3,4-tetrahydro-6-hydroxy-2-naphthalenecarbonyl-L-alanyl-L-alanyl-L-alanyl-L-alanyl-2-methylalanyl-L-alanyl-N-(4-iodophenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

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PAGE 1-B

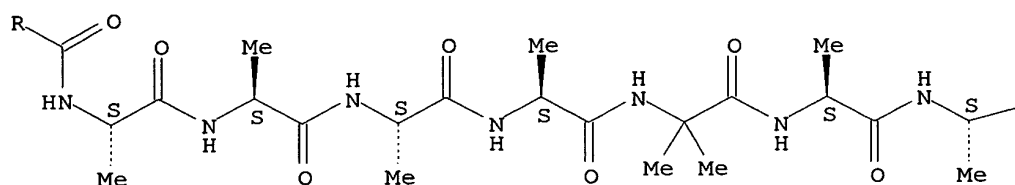
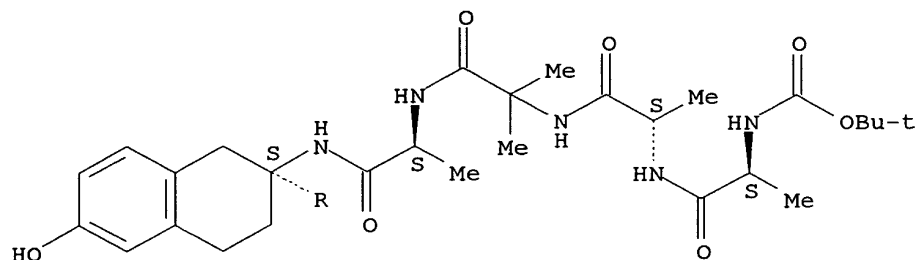


RN 197431-13-3 CAPLUS

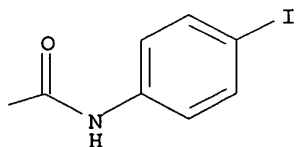
CN L-Alaninamide, N-[(1,1-dimethylethoxy)carbonyl]-L-alanyl-L-alanyl-2-methylalanyl-L-alanyl-(2S)-2-amino-1,2,3,4-tetrahydro-6-hydroxy-2-naphthalenecarbonyl-L-alanyl-L-alanyl-L-alanyl-L-alanyl-2-methylalanyl-L-alanyl-N-(4-iodophenyl)-, monohydrate (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

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PAGE 1-B

● H<sub>2</sub>O

L5 ANSWER 4 OF 8 CAPLUS COPYRIGHT 2000 ACS

ACCESSION NUMBER: 1996:741618 CAPLUS

DOCUMENT NUMBER: 126:89768

TITLE: A small library of peptidomimetics to systematically vary and test the effects of x1 constraints

AUTHOR(S): Burgess, Kevin; Godbout, Claude; Li, Wen; Payza, Kemal

CORPORATE SOURCE: Department Chemistry, Texas A &amp; M University, College Station, TX, 77843-3255, USA

SOURCE: Bioorg. Med. Chem. Lett. (1996), 6(22), 2761-2764

CODEN: BMCLE8; ISSN: 0960-894X

PUBLISHER: Elsevier

DOCUMENT TYPE: Journal

Searched by Barb O'Bryen, STIC 308-4291

LANGUAGE: English

AB A library of 47 peptidomimetics of H-Tyr-Gly-Gly-Phe-Leu-Arg-Phe-NH<sub>2</sub> was prepd. wherein 32 of these contained one of the four different isomers of the conformationally constrained 2,3-methanoleucine for Leu5. This library was tested for binding the neuropeptide FF receptor where neuropeptide FF is H-Phe-Leu-Phe-Gln-Pro-Gln-Arg-Phe-NH<sub>2</sub>, an anti-opiate peptide. This study illustrates how conformational constraints can be systematically varied in a library format to det. the best conformational restrictions for the desired activity.

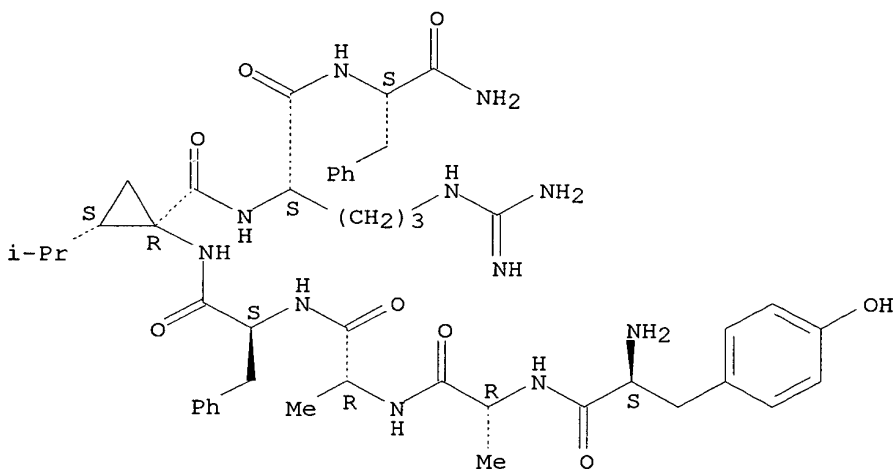
IT 185751-47-7P 185751-51-3P 185751-55-7P  
185751-59-1P 185751-63-7P 185751-67-1P  
185751-71-7P 185751-75-1P

RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)  
(prepn. of a peptidomimetic library contg. conformationally constrained methanoleucine)

RN 185751-47-7 CAPLUS

CN L-Phenylalaninamide, L-tyrosyl-D-alanyl-D-alanyl-L-phenylalanyl-(1R,2S)-1-amino-2-(1-methylethyl)cyclopropanecarbonyl-L-arginyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

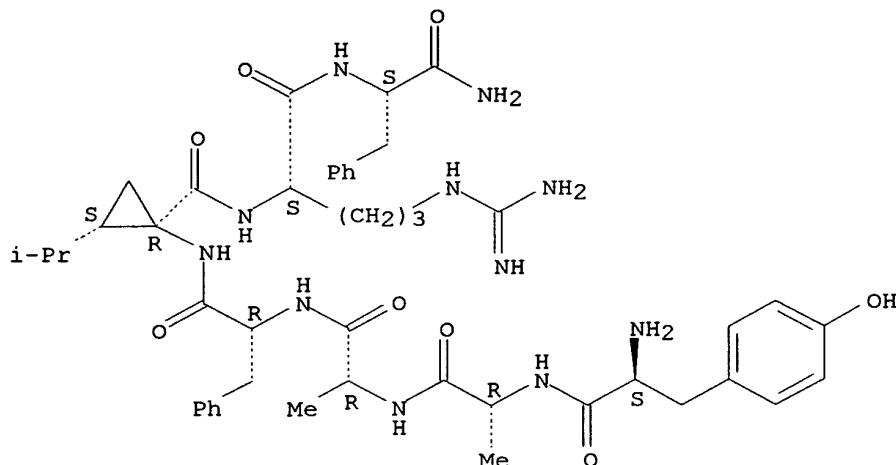


RN 185751-51-3 CAPLUS

CN L-Phenylalaninamide, L-tyrosyl-D-alanyl-D-alanyl-D-phenylalanyl-(1R,2S)-1-amino-2-(1-methylethyl)cyclopropanecarbonyl-L-arginyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

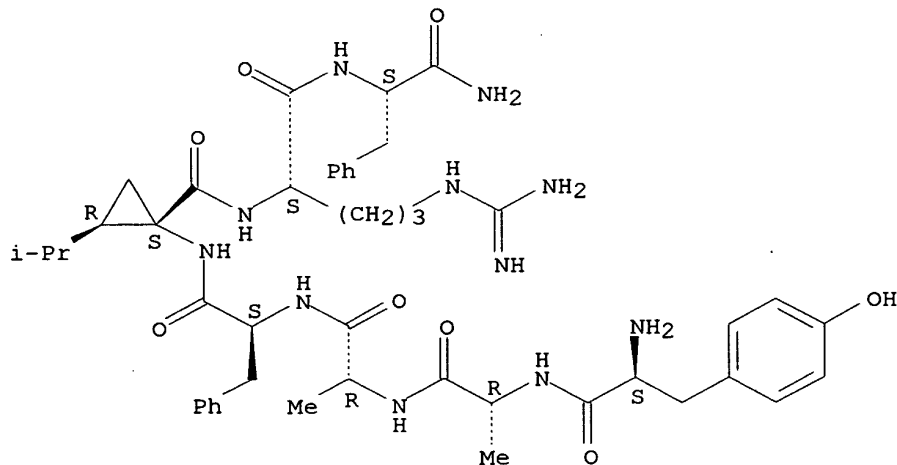




RN 185751-55-7 CAPLUS

CN L-Phenylalaninamide, L-tyrosyl-D-alanyl-D-alanyl-L-phenylalanyl-(1S,2R)-1-amino-2-(1-methylethyl)cyclopropanecarbonyl-L-arginyl- (9CI) (CA INDEX NAME)

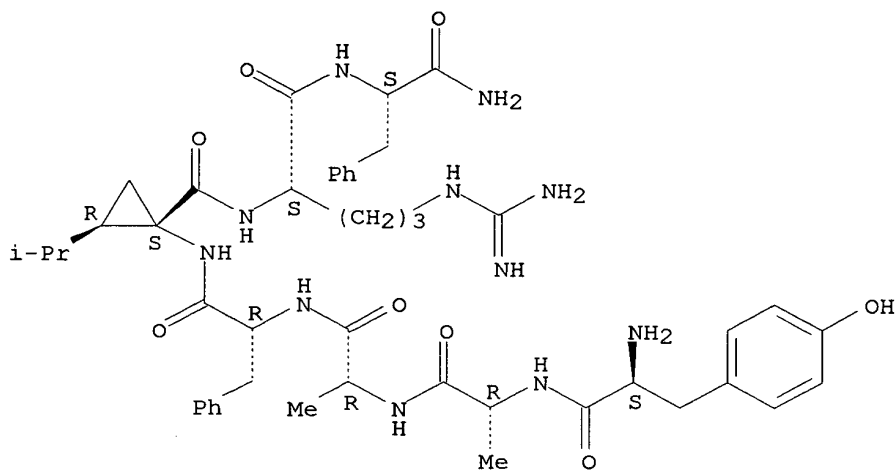
Absolute stereochemistry.



RN 185751-59-1 CAPLUS

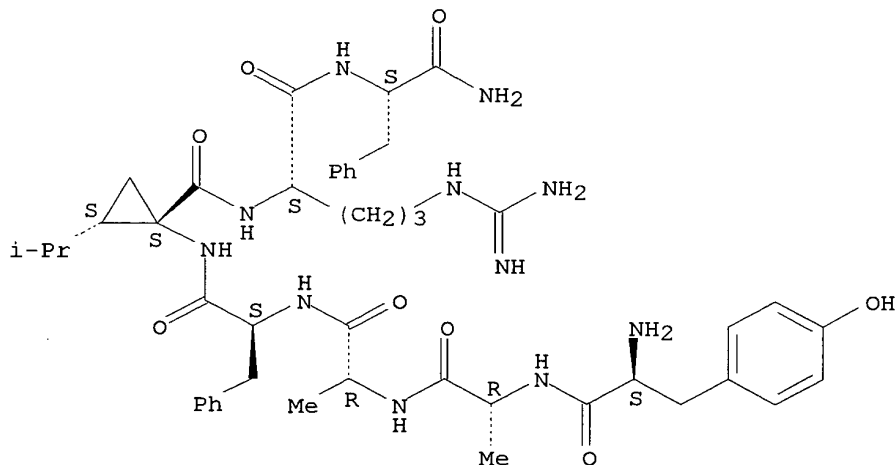
CN L-Phenylalaninamide, L-tyrosyl-D-alanyl-D-alanyl-D-phenylalanyl-(1S,2R)-1-amino-2-(1-methylethyl)cyclopropanecarbonyl-L-arginyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



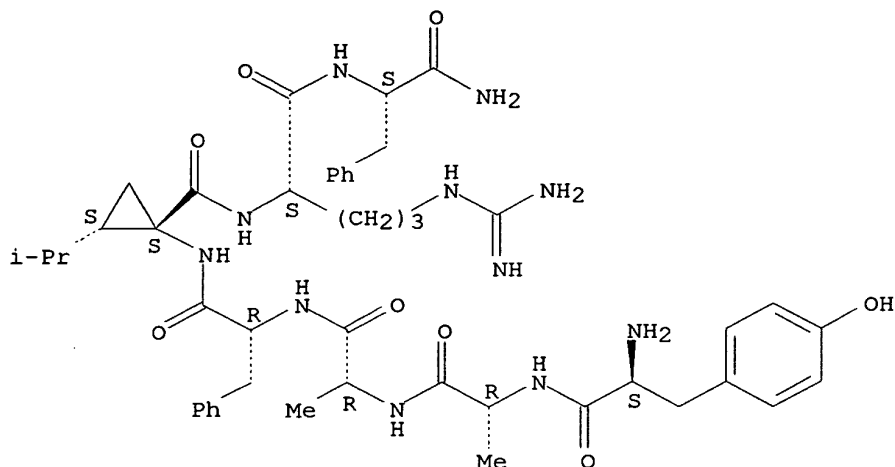
RN 185751-63-7 CAPLUS  
 CN L-Phenylalanyl-L-tyrosyl-D-alanyl-D-alanyl-L-phenylalanyl-(1S,2S)-1-amino-2-(1-methylethyl)cyclopropanecarbonyl-L-arginyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 185751-67-1 CAPLUS  
 CN L-Phenylalanyl-L-tyrosyl-D-alanyl-D-alanyl-D-phenylalanyl-(1S,2S)-1-amino-2-(1-methylethyl)cyclopropanecarbonyl-L-arginyl- (9CI) (CA INDEX NAME)

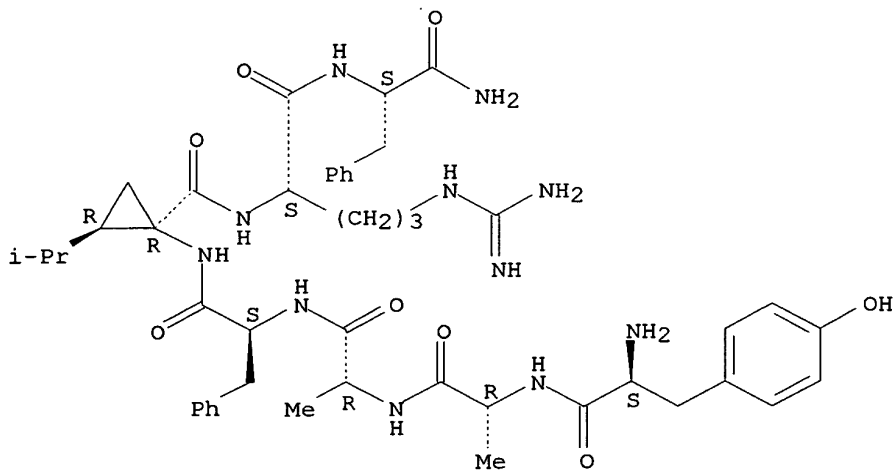
Absolute stereochemistry.



RN 185751-71-7 CAPLUS

CN L-Phenylalaninamide, L-tyrosyl-D-alanyl-D-alanyl-L-phenylalanyl-(1R,2R)-1-amino-2-(1-methylethyl)cyclopropanecarbonyl-L-arginyl- (9CI) (CA INDEX NAME)

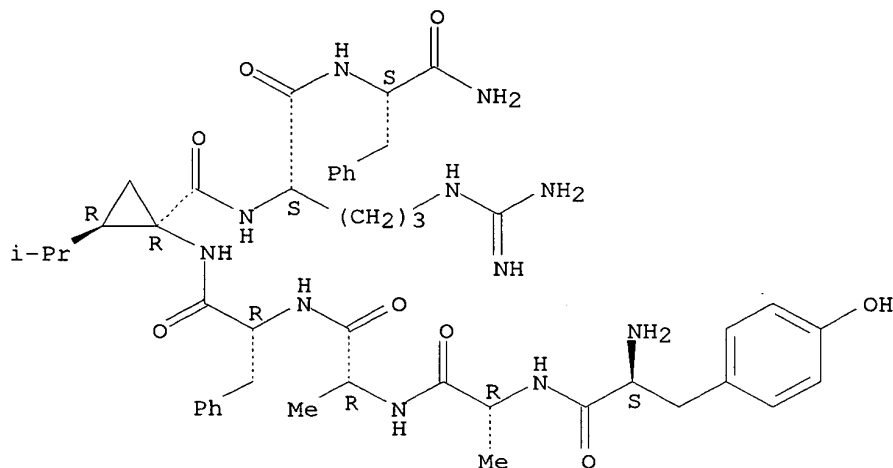
Absolute stereochemistry.



RN 185751-75-1 CAPLUS

CN L-Phenylalaninamide, L-tyrosyl-D-alanyl-D-alanyl-D-phenylalanyl-(1R,2R)-1-amino-2-(1-methylethyl)cyclopropanecarbonyl-L-arginyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 5 OF 8 CAPLUS COPYRIGHT 2000 ACS

ACCESSION NUMBER: 1995:846974 CAPLUS

DOCUMENT NUMBER: 123:257365

TITLE: .alpha.-Helical versus 310-Helical Conformation of Alanine-Based Peptides in Aqueous Solution: An Electron Spin Resonance Investigation

AUTHOR(S): Smythe, Mark L.; Nakaie, Clovis R.; Marshall, Garland R.

CORPORATE SOURCE: School of Medicine, Washington University, St. Louis, MO, 63110, USA

SOURCE: J. Am. Chem. Soc. (1995), 117(42), 10555-62

CODEN: JACSAT; ISSN: 0002-7863

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 123:257365

AB Due to the difficulties in exptl. differentiating between the .alpha.- and 310-helical conformations in soln., isolated peptides were assumed to be in the .alpha.-helical conformation. However, recent ESR studies have suggested that such peptides, in particular short alanine-based peptides, are 310-helical (Miick, S. M.; et al. 1992). This result prompted the authors to further investigate the helical conformations of alanine-based peptides in soln. using ESR. Unlike previous investigations with a flexible link connecting the spin-label to the peptide backbone, the authors used a conformationally constrained spin-label (4-amino-4-carboxy-2,2,6,6-tetramethylpiperidine-1-oxyl, Toac) that is rigidly attached to the peptide backbone. From a combination of mol. modeling and ESR spectroscopy investigations, it was concluded that these alanine-based peptides exist primarily in the .alpha.-helical conformation, and not the 310-form as previously suggested for an analogous set of peptides in aq. environments. This discrepancy is thought to be due to the differences in flexibility of the spin-labels employed. The conformationally constrained spin-label Toac used in this study should accurately reflect the backbone conformation. Free energy surfaces, or potentials of mean force, for the conformational transition of the spin-label used in previous studies (Miick S. M.; et al. 1992) suggest that this spin-label is too flexible to accurately distinguish between the .alpha.- and 310-helical conformations.

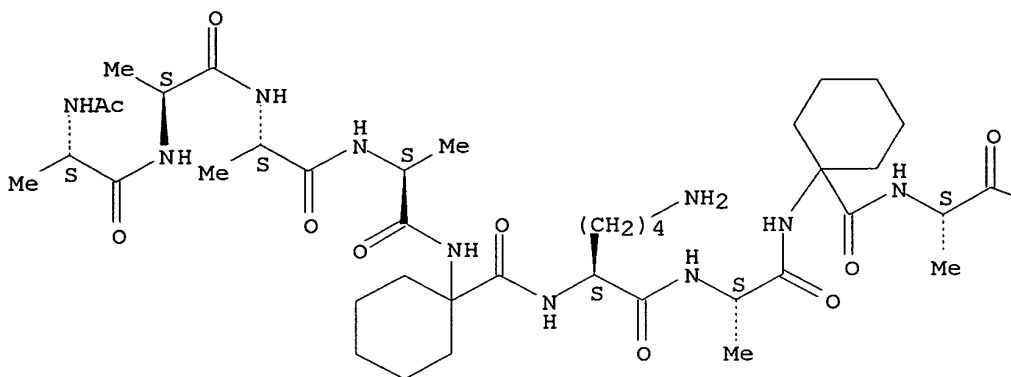
IT 169134-77-4P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
(.alpha.-helical vs. 310-helical conformation of alanine-based peptides  
Searched by Barb O'Bryen, STIC 308-4291

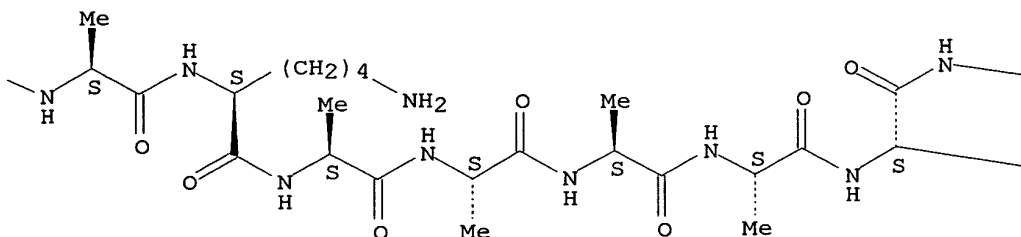
RN 169134-77-4 CAPLUS

CN L-Alaninamide, N-acetyl-L-alanyl-L-alanyl-L-alanyl-L-alanyl-1-aminocyclohexanecarbonyl-L-lysyl-L-alanyl-1-aminocyclohexanecarbonyl-L-alanyl-L-alanyl-L-lysyl-L-alanyl-L-alanyl-L-alanyl-L-alanyl-L-lysyl- (9CI)  
 (CA INDEX NAME)

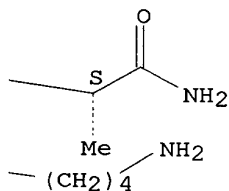
PAGE 1-A



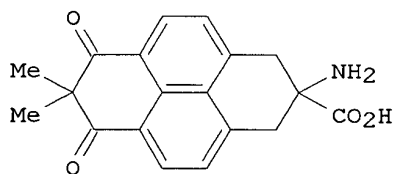
PAGE 1-B



PAGE 1-C



L5 ANSWER 6 OF 8 CAPLUS COPYRIGHT 2000 ACS  
 ACCESSION NUMBER: 1995:380710 CAPLUS  
 DOCUMENT NUMBER: 122:161358  
 TITLE: Helical Stability of de Novo Designed  
 .alpha.-Aminoisobutyric Acid-Rich Peptides at High  
 Temperatures  
 AUTHOR(S): Augspurger, J. D.; Bindra, V. A.; Scheraga, H. A.;  
 Kuki, A.  
 CORPORATE SOURCE: Baker Laboratory of Chemistry, Cornell University,  
 Ithaca, NY, 14853-1301, USA  
 SOURCE: Biochemistry (1995), 34(8), 2566-76  
 CODEN: BICHAW; ISSN: 0006-2960  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 GI



I

AB 1- And 2-dimensional NMR spectroscopy is used to det. the helical stability of two Aib-rich peptides, Me<sub>2</sub>CHCH<sub>2</sub>CO<sub>2</sub>C-(Aib)<sub>3</sub>-DkNap-Leu-Aib-Ala-(Aib)<sub>2</sub>-NHCH<sub>2</sub>CH<sub>2</sub>OMe (DkNap = phenylenedione-based amino acid I) (Dk4[7/9]) and Ac-(Aib)<sub>2</sub>-Nap-(Aib)<sub>2</sub>-Phe-(Aib)<sub>2</sub>-NHMe [Nap = .beta.-(1-naphthyl)-L-alanine] (Nap3Phe6[6/8]), where the bracket notation indicates the no. of Aib-class residues/total no. of residues. 2D ROESY expts., carried out previously on Nap3Phe6[6/8] in DMSO (Basu, G., & Kuki, A. 1993), showed that this compd. adopts the 310-helical conformation at 20 .degree.C. The first step in the present work is to apply this technique to the peptide Dk4[7/9], demonstrating that it likewise adopts the 310-helical conformation in chloroform at 20.degree.. The amide proton shifts of Nap3Phe6[6/8] in DMSO and Dk4[7/9] in C<sub>2</sub>D<sub>2</sub>Cl<sub>4</sub> were then monitored by 1-dimensional NMR over a large temp. range, up to 150 and 120.degree., resp. The nonamer Dk4[7/9] exhibits no evidence of any conformational or unfolding transition as the temp. is raised. The nearly temp. independent amide proton chem. shifts of this nonamer are an indication of retention of the intrahelical hydrogen bonding, which was then verified directly by solvent perturbation with DMSO at 120.degree.. The resulting

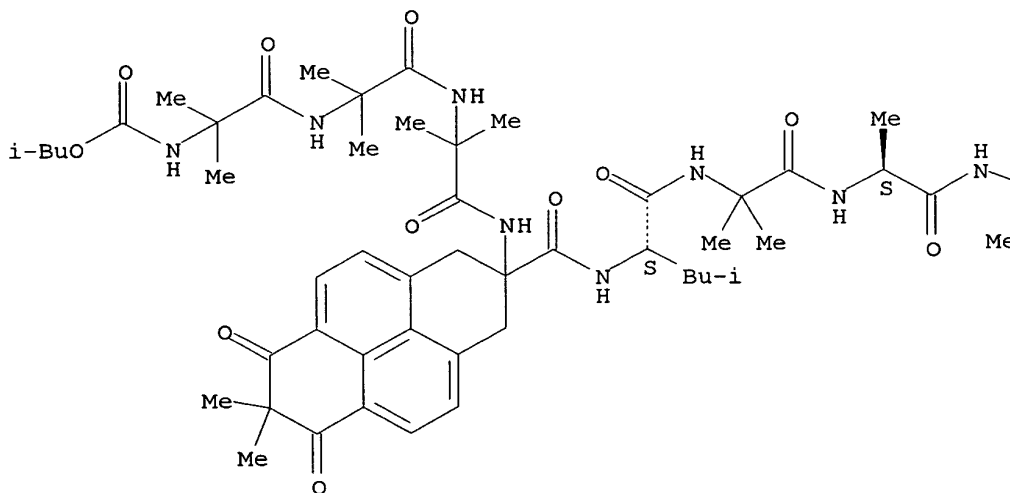
Searched by Barb O'Bryen, STIC 308-4291

IT 157662-09-4

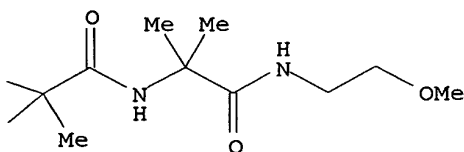
(helical stability of de novo designed .alpha.-aminoisobutyric acid-rich peptides at high temps.)

157862 85 1 CH 255  
 CN Alaninamide, 2-methyl-N-[(2-methylpropoxy)carbonyl]alanyl-2-methylalanyl-2-  
 pyrenecarboxyl-1,2,3,6,7,8-hexahydro-7,7-dimethyl-6,8-dioxo-2-amino-2-  
 pyrenecarboxyl-L-leucyl-2-methylalanyl-L-alanyl-2-methylalanyl-N-(2-  
 methoxyethyl)-2-methyl- (9CI) (CA INDEX NAME)

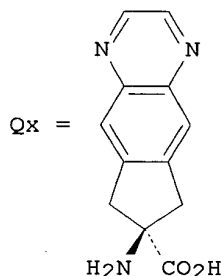
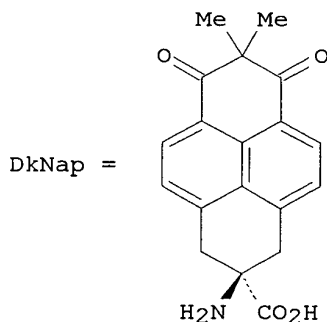
PAGE 1-A



PAGE 1-B



ACCESSION NUMBER: 1995:285530 CAPLUS  
 DOCUMENT NUMBER: 122:161342  
 TITLE: Conformational preferences of oligopeptides rich in  
 .alpha.-aminoisobutyric acid. III. Design, synthesis  
 and hydrogen bonding in 310-helices  
 AUTHOR(S): Bindra, Vandana A.; Kuki, Atsuo  
 CORPORATE SOURCE: Dep. Chem. Baker Lab., Cornell Univ., Ithaca, NY, USA  
 SOURCE: Int. J. Pept. Protein Res. (1994), 44(6), 539-48  
 CODEN: IJPPC3; ISSN: 0367-8377  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 GI

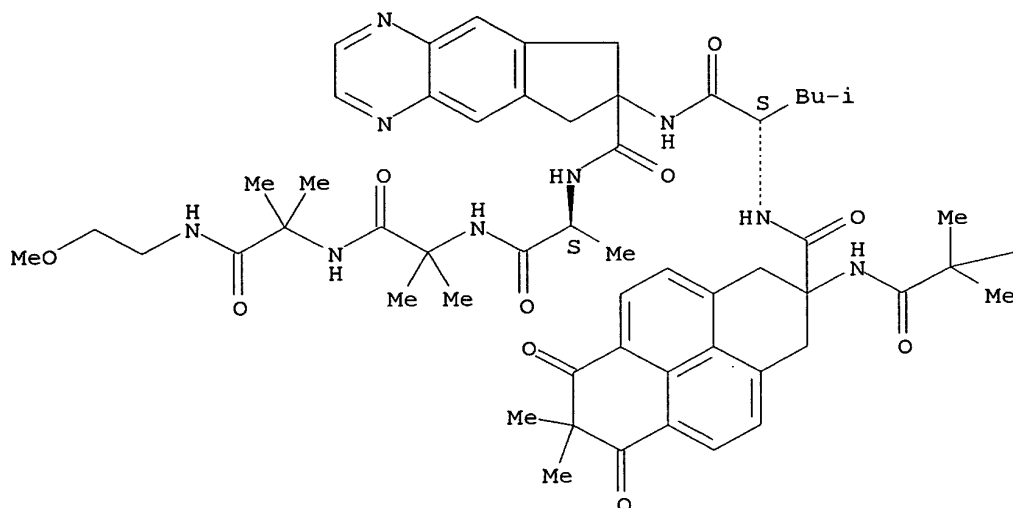


- AB Two sterically constrained peptides, iBoc-(Aib)<sub>3</sub>-DkNap-Leu-X-Ala-Aib-Aib-Fl (I; Aib = .alpha.-aminoisobutyric acid; Fl = NHCH<sub>2</sub>CH<sub>2</sub>OMe; iBoc = Me<sub>2</sub>CHCH<sub>2</sub>O<sub>2</sub>C; X = Aib, Qx), contg. Aib and Aib-class amino acids in conjunction with selected mono-.alpha.-alkyl amino acids were synthesized by an optimized procedure. The use of Aib-class amino acids DkNap and Qx gives rise to the same overwhelmingly 310-helical backbone conformation as that provided by simpler Aib-rich peptides and homopeptides. The synthetic .alpha.,.alpha.-dialkylamino acids DkNap and Qx are arom. homologues of the known alicyclic variants of Aib, the Ac5c and Ac6c amino acids. Two new org. solubilizing groups for peptides, iBoc and Fl, are introduced. The 1H NMR analyses of I demonstrate the unambiguous 210-helical hydrogen bonding pattern of these peptides, confirming the design objective of these sequence patterns contg. greater than 50% Aib and Aib-class compn.
- IT **157662-08-3P 157662-09-4P**  
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
 (design, synthesis, and hydrogen bonding in 310-helical .alpha.-aminoisobutyric acid-contg. peptides and analogs)
- RN 157662-08-3 CAPLUS
- CN Alaninamide, 2-methyl-N-[(2-methylpropoxy)carbonyl]alanyl-2-methylalanyl-2-methylalanyl-1,2,3,6,7,8-hexahydro-7,7-dimethyl-6,8-dioxo-2-amino-2-pyrenecarbonyl-L-leucyl-7,8-dihydro-7-amino-6H-cyclopenta[g]quinoxaline-7-carbonyl-L-alanyl-2-methylalanyl-N-(2-methoxyethyl)-2-methyl- (9CI) (CA INDEX NAME)

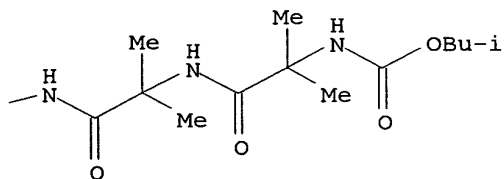
Absolute stereochemistry.



PAGE 1-A



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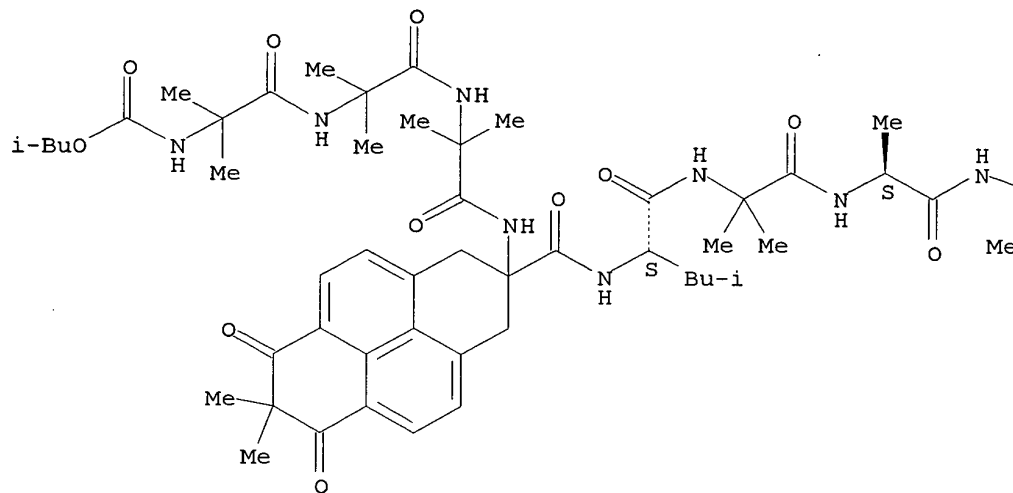


RN 157662-09-4 CAPLUS

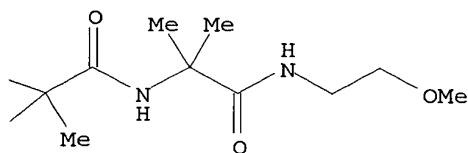
157662-69-4    CA1635  
 CN    Alaninamide, 2-methyl-N-[(2-methylpropoxy)carbonyl]alanyl-2-methylalanyl-2-methylalanyl-1,2,3,6,7,8-hexahydro-7,7-dimethyl-6,8-dioxo-2-amino-2-pyrenecarbonyl-L-leucyl-2-methylalanyl-L-alanyl-2-methylalanyl-N-(2-methoxyethyl)-2-methyl- (9CI)    (CA INDEX NAME)

Absolute stereochemistry.

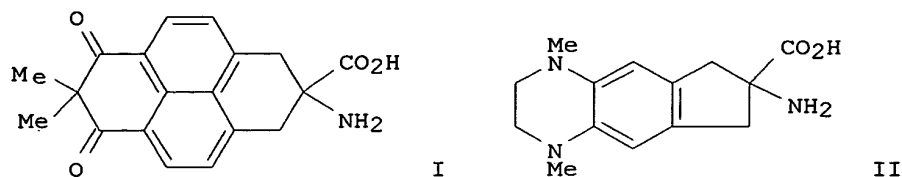
PAGE 1-A



PAGE 1-B



L5 ANSWER 8 OF 8 CAPLUS COPYRIGHT 2000 ACS  
ACCESSION NUMBER: 1994:580159 CAPLUS  
DOCUMENT NUMBER: 121:180159  
TITLE: Photoinduced electron transfer and long-lived charge separation in rigid peptide architectures  
AUTHOR(S): Anglos, Demetrios; Bindra, Vandana; Kuki, Atsuo  
CORPORATE SOURCE: Dep. Chem., Cornell Univ., Ithaca, NY, 14853-1301, USA  
SOURCE: J. Chem. Soc., Chem. Commun. (1994), (2), 213-15  
CODEN: JCCCAT; ISSN: 0022-4936  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
GI



AB Phenylenedione-based amino acid I (DkNap) and tetrahydroquinoxaline-based amino acid II (ThQx) were used to construct two novel architectures, cyclo(DkNap-ThQx) and helical .alpha.-aminoisobutyric acid (Aib)-rich nonapeptide Me<sub>2</sub>CHCH<sub>2</sub>O<sub>2</sub>C-(Aib)<sub>3</sub>-DkNap-Leu-ThQx-Ala-(Aib)<sub>2</sub>-NHCH<sub>2</sub>CH<sub>2</sub>OMe, providing a rigid structural framework for the study of intramol., photoinduced electron transfer between the two custom-designed donor-acceptor redox .alpha.-amino acids.

IT 157662-08-3 157662-09-4

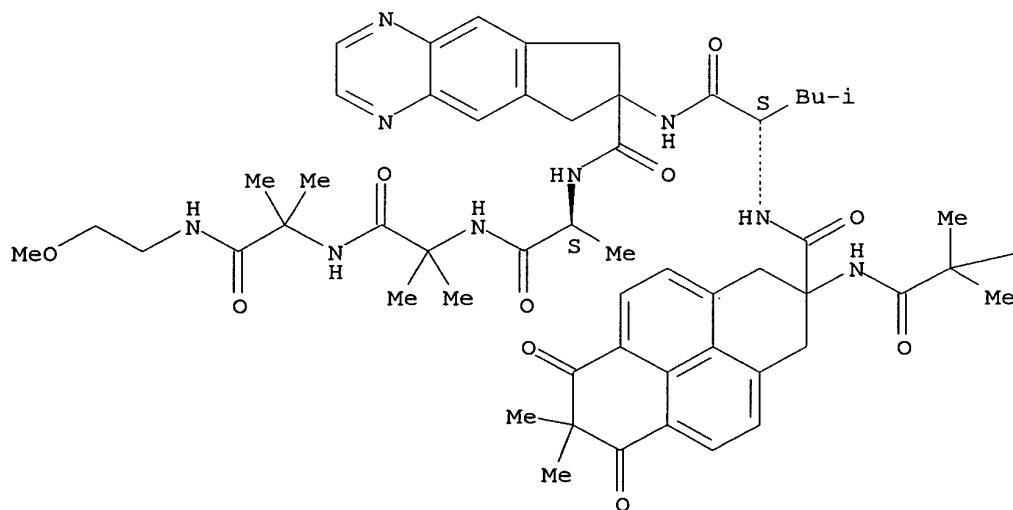
RL: PRP (Properties)  
(conformation of, by NMR)

RN 157662-08-3 CAPLUS

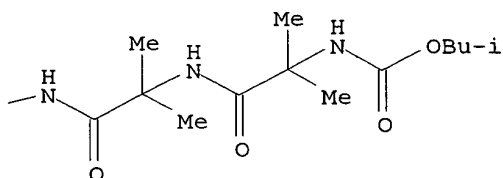
CN Alaninamide, 2-methyl-N-[(2-methylpropoxy)carbonyl]alanyl-2-methylalanyl-2-methylalanyl-1,2,3,6,7,8-hexahydro-7,7-dimethyl-6,8-dioxo-2-amino-2-pyrenecarbonyl-L-leucyl-7,8-dihydro-7-amino-6H-cyclopenta[g]quinoxaline-7-carbonyl-L-alanyl-2-methylalanyl-N-(2-methoxyethyl)-2-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

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PAGE 1-B

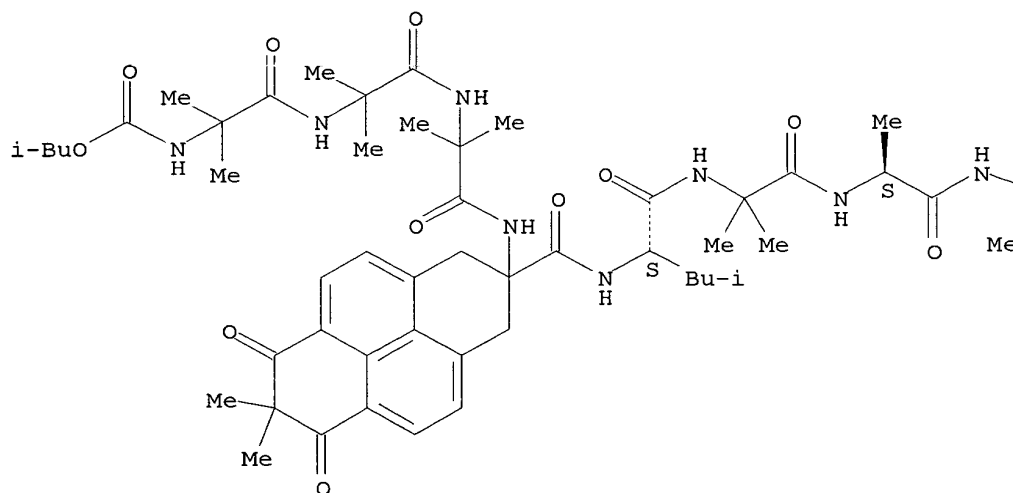


RN 157662-09-4 CAPLUS

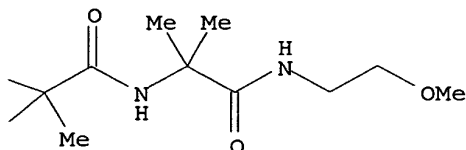
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Absolute stereochemistry.

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PAGE 1-B



IT 157662-07-2P

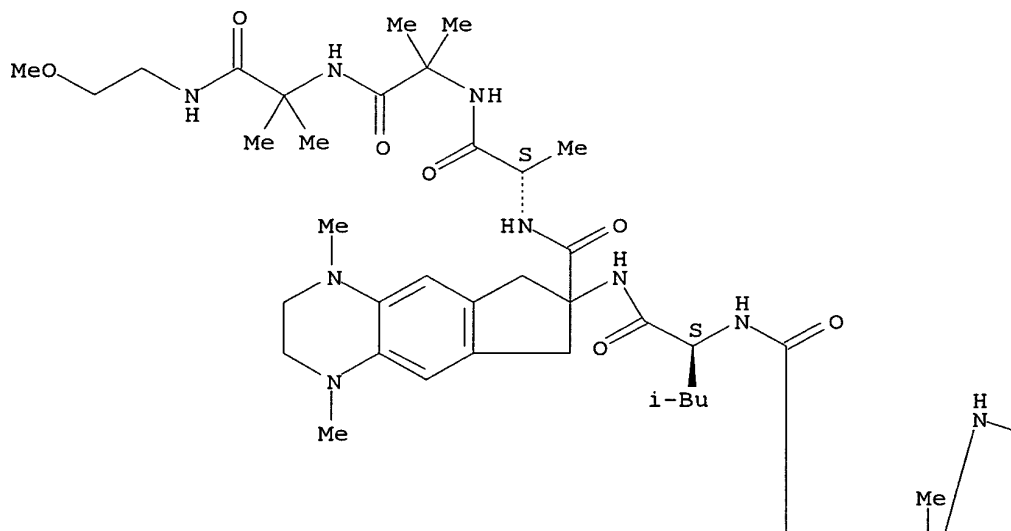
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(prepn., conformation, and intramol. photoinduced electron transfer of)

RN 157662-07-2 CAPLUS

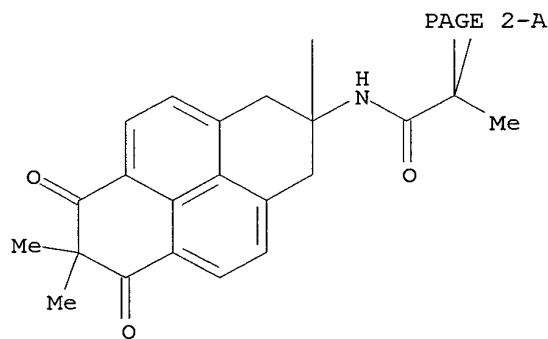
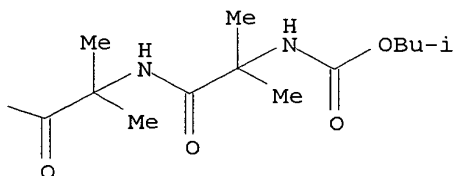
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Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



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